PR-4. DESIGN AND PHOTOPHYSICS OF 2-VINYL QUINAZOLIN-4-ONES

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Quinazoline derivatives are coming to sustained fame in the last couple of decades experienced predominantly as a rapid growth in the search of new photoelectronic materials [1], as well as of new drugs, and biomedical indicators up to potential gene engineering tools [2]. This report presents our initial photophysical results on a series of 2-substituted quinazolin-4-ones designed to be capable of intramolecular proton transfer in the ground and/or the excited electronic state, (ES)IPT. The molecules are usually tautomeric in the ground electronic state [3] and can form chelate complexes with metal cations or boron fluoride. The resulting BODIPY® dyes in the latter case are among the ultimate goals of our design.

The structural novelty we use in the search of quinazoline chromophores and fluorophores is closely related to the search of heterocyclic ligands capable to extend the field of borofluoride dyes [4], considered to derive from ESIPT molecules [5]. As the photophysics of the latter shows substantial solvent vibronic effects [5], it is of particular interest to follow the possible transfer of spectroscopic properties to the related BF_2 complexes first in theory by computation, and then in experiment. Specifically, as boron contribution to the conjugated π-electron system of a chromophore or fluorophore is a π-electron hole, minimal changes in electronic spectra should not come as a surprise.

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